SESSION J13: DMP: THEORY OF MATERIALS
Wednesday morning, 24 March 1993; Room 211 at 11:00 G. Baraff, presiding

Invited Papers

11:00

J13 1 Chemical-Potential Dependence of Impurity and Defect-Formation Energies in GaAs.*

SHENG-BAI ZHANG, National Renewable Energy Laboratory.

Recent experiments and theoretical studies both point to the direction that the absolute formation energy and hence the equilibrium concentration of defects and impurities in GaAs depends strongly on the atomic chemical potentials of As and Ga as well as the electron chemical potential. For example, (1) *ab initio* calculations showed that the equilibrium Ga vacancy concentration changes by more than 10 orders of magnitude as the chemical potentials of As and **Ga vary** over the thermodynamically allowed range. This result indicates that the rate of Ga self-diffusion depends strongly on the surface-annealing conditions. (2) By calculating the formation energy of Si donors, acceptors and defect complexes, the equilibrium concentrations of native defects and Si-defect complexes as well as the total solubility of Si in GaAs were determined. The calculated solubiity limit is in good agreement with experiment. A Si-vacancy complex ($[Si_{Ga} - V_{Ga}]^{2-}$) occurs in relatively high concentration under As-rich conditions and may therefore mediate Si and **Ga** diffusion. This complex also provides an important mechanism for compensation in heavily doped GaAs.

‘This work was performed at Xerox PARC in collaboration with J. E. Northrup.